

Two-electron quantum dot model revisited: bound states and other analytical and numerical solutions

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Abstract

The model of a two-electron quantum dot, confined to move in a two dimensional flat space, is revisited. Generally, it is argued that the solutions of this model obtained by solving a biconfluent Heun equation have some limitations. In particular, some corrections are also made in previous theoretical calculations. The corrected polynomial solutions are confronted with numerical calculations based on the Numerov method, in a good agreement between both. Then, new solutions considering the $1/r$ and $\ln r$ Coulombian-like potentials in $(1+2)D$, not yet obtained, are discussed numerically. In particular, we are able to calculate the quantum dot eigenfunctions for a much larger spectrum of external harmonic frequencies as compared to previous results. Also the existence of bound states for such planar system in the case $l = 0$ is predicted and the respective eigenvalues are determined.

Keywords: Schrödinger equation, two-electron system, quantum dot model, Numerov numerical method, Heun's equation

1. Introduction

Modern technics in nanometer-scale semiconductor manufacturing enable the creation of quantum confinement of only a few electrons. These few-body systems are often called quantum dots [1]. They can be described by a model where the electrons move in an external harmonic oscillator potential of frequency Ω , exhibiting a two dimensional behavior [2]. Previous numerical

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calculations suggest that the harmonic oscillator potential can be successfully employed to describe two-electron quantum dot [3]. Thus, a model for this kind of system can be described by the time independent Schrödinger equation, in atomic units ($\hbar = m = e = 1$),

$$\left\{ -\frac{1}{2}(\vec{\nabla}_1^2 + \vec{\nabla}_2^2) + \frac{\Omega^2}{2}(r_1^2 + r_2^2) + \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right\} \Psi(\vec{r}_1, \vec{r}_2) = E_T \Psi(\vec{r}_1, \vec{r}_2) \quad (1)$$

where the subscripts 1 and 2 refer to each one of the electrons. The \vec{r}_i are two-dimensional vectors with length $r_i = |\vec{r}_i|$. Introducing the usual relative and center of mass coordinates, $\vec{r} = \vec{r}_1 - \vec{r}_2$ and $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$, Eq. (1), with the choice $\Psi(\vec{r}_1, \vec{r}_2) = \chi(\vec{R})\psi(\vec{r})$, gives rise to the following relative coordinate equation:

$$\left[-\nabla_{\vec{r}}^2 + \omega^2 r^2 + \frac{1}{r} \right] \psi(\vec{r}) = \eta \psi(\vec{r}) \quad (2)$$

where one has defined the frequency $\omega = \Omega/2$. The total energy is given by $E_T = \epsilon + \eta$, with ϵ being the center of mass amount of energy.

The 2D radial Schrödinger equation for the relative coordinate can be obtained by introducing the polar coordinates (r, θ) and putting its solution in the form

$$\psi(\vec{r}) = r^{-1/2} u(r) e^{\pm i l \theta} \quad (3)$$

where l is the integer angular momentum quantum number of the two-dimensional system. The radial function $u(r)$ should satisfy the following equation:

$$\frac{d^2 u(r)}{dr^2} + \left[\eta - \frac{1}{r} - \omega^2 r^2 - \frac{(l^2 - 1/4)}{r^2} \right] u(r) = 0 \quad (4)$$

The problem of two electrons in an external oscillator potential is studied in three dimensions [4], and it is shown that the above radial equation is *quasi-exactly solvable* [5, 6, 7], which means that it is possible to find exact simple solutions for some, but not all, eigenfunctions, corresponding to a certain infinite set of discrete oscillator frequencies. In a recent paper [8], it was shown that it is possible to determine exactly and in a closed form a finite portion of the energy spectrum and the associated eigenfunctions for the Schrödinger equation describing the relative motion of a two-electron system, by putting Eq. (4) into the form of a biconfluent Heun equation, like

$$x y''(x) + [1 + \alpha - 2x^2] y' + [-\delta/2 + (\gamma - \alpha - 2)x] y(x) = 0 \quad (5)$$

where

$$\alpha = 2l; \quad \gamma = \frac{\eta}{\omega}; \quad \delta = \frac{2}{\sqrt{\omega}} \quad (6)$$

and the relation between the functions $u(r)$ and $y(x)$, with $x = \sqrt{\omega}r$, is given by

$$u(r) = r^{l+1/2} e^{-\omega r^2/2} y(\sqrt{\omega}r) \quad (7)$$

The first scope of this paper is to correct some details in the analytical calculation of Ref. [8], as discussed in Section 2. The particular solutions obtained by analytically solving the Biconfluent Heun Equations (BHE) form a set of solutions just for a discrete set of external frequencies Ω . This method, indeed, did not give us a polynomial solution for any frequency Ω . Each solution is obtained for a specific frequency value. The same is true for other studies [9, 10, 11]. Therefore, it is natural to wonder if a numerical analysis of this problem could give rise to a broad class of solutions well defined for just one frequency external value Ω as it is expected in a real experimental situation. That brings us to the second scope, namely to solve numerically the Schrödinger radial equation, Eq. (4), by using the Numerov method [12]. This will open new possibilities: that of calculating the bound-state solutions for the two-electron quantum dots; that of checking the previous analytical results; that of finding new states for arbitrary Ω values; and finally that of investigating the difference on both the eigenvalues and eigenfunctions by changing the Coulombian potential from $1/r$ to $\ln r$, as is expected for a strictly two-dimensional system.

2. Polynomial solutions revisited

The energy spectrum and the associated eigenfunctions for the radial Schrödinger equation, Eq. (4), describing the relative motion of the two electrons, were obtained by putting it into the form of a Biconfluent Heun equation [8]. However, two corrections should be considered. First of all, in the Eq. (4) the term containing the energy η appeared multiplied by a factor 2 in that paper. The second error there is that the authors took the parameter α from the book [14], which is not correct, and this implies the γ factor is also wrong. The corrected values are already given in Eq. (6).

Taking these corrections into account, the polynomial solutions of Eq. (5),

when α is not a negative integer, can be written as

$$y(x) = N(\alpha, 0, \gamma, \delta; x) = \sum_{p=0}^{\infty} \frac{A_p}{(1+\alpha)_p} \frac{x^p}{p!} \quad (8)$$

with

$$(\alpha)_p = \frac{\Gamma(\alpha + p)}{\Gamma(\alpha)}, \quad p \geq 0$$

The two first coefficients are $A_0 = 1$ and $A_1 = \delta/2$. To simplify we will use $\delta' \equiv -\delta/2$, and the others coefficients can be determined by:

$$(\gamma - \alpha - 2 - 2p)(p+1)(p+\alpha+1)A_p + \delta' A_{p+1} + A_{p+2} = 0$$

The first consequence of this recurrence formula is that the solution of Eq. (5) becomes a polynomial of degree n if and only if

$$\gamma - \alpha - 2 = 2n \quad \Rightarrow \quad \eta_{nl} = 2(n+l+1)\omega \quad (9)$$

which is a quantum condition between the energy η_{nl} and the frequency ω . This result brings an extra overall factor 2 for the energy if compared to the equivalent result of Ref. [8].

Notice that now A_n is a polynomial in $1/\sqrt{\omega}$. There is at most n suitable values of $1/\sqrt{\omega}$. These roots can be named $(\delta')_{\mu}^n$, with $0 \leq \mu \leq n$. All these roots denoted by $1/\sqrt{\omega_{nl}}$ are given in Table 1 for values from $n = 1$ to $n = 5$ and the respective range of l .

Similarly to Ref. [11], for even values of n we find solutions corresponding to the limit $\omega \rightarrow \infty$ ($1/\sqrt{\omega} \rightarrow 0$), which was called an asymptotic solution.

Once the roots are determined, one can compute the energy levels and write down, from Eq. (8), the explicit form of the functions y_{nl} ($1 \leq n \leq 5$).

For $l = 0$, the polynomials are explicitly given by:

$$\begin{aligned} y_{10} &= 1 + r \\ y_{20} &= 1 + r + 0.1667 r^2 \\ y_{30} &= 1 + r + 0.2096 r^2 + 0.1079 r^3 \\ y_{40} &= 1 + r + 0.2263 r^2 + 0.2124 r^3 + 0.0004 r^4 \\ y_{50} &= 1 + r + 0.1945 r^2 + 0.1041 r^3 - 0.0015 r^4 - 0.00007 r^5 \end{aligned}$$

Remembering that

$$u_{nl} = r^{l+1/2} e^{-\omega_{nl} r^2/2} y_{nl}(r)$$

Table 1: Some roots of $1/\sqrt{\omega_{nl}}$ for different values of n and l .

n	l	$1/\sqrt{\omega_{nl}}$
1	0	$\sqrt{2}$
2	0	$\sqrt{12}$
	1	$\sqrt{28}$
3	0	1.7064561; 6.0899924
	1	2.7280686; 8.5180773
	2	3.4097585; 10.4102615
4	0	3.9411450; 9.1906134
	1	5.7789370; 12.1080092
	2	7.0834449; 14.4853307
	3	8.1607519; 16.5348760
5	0	1.9283; 6.7103
	1	2.9566; 9.1687
	2	3.6224; 11.029
	3	4.1621; 12.592
	4	4.6313; 13.970

then, from the roots of Table 1, we can get the following expressions for the wave-functions:

$$\begin{aligned}
u_{10} &= r^{\frac{1}{2}} e^{-0.25 r^2} [1 + r] \\
u_{20} &= r^{\frac{1}{2}} e^{-0.0417 r^2} [1 + r + 0.1667 r^2] \\
u_{30} &= r^{\frac{1}{2}} e^{-0.0135 r^2} [1 + r + 0.2096 r^2 + 0.1079 r^3] \\
u_{40} &= r^{\frac{1}{2}} e^{-0.0059 r^2} [1 + r + 0.2263 r^2 + 0.2124 r^3 + 0.0004 r^4] \\
u_{50} &= r^{\frac{1}{2}} e^{-0.0111 r^2} [1 + r + 0.1945 r^2 + 0.1041 r^3 - 0.0015 r^4 - 0.00007 r^5]
\end{aligned}$$

These states are shown in arbitrary units in Fig. 1.

As the last remark of this Section, we would like to stress that in addition to the roots shown in Table 1 we have found, for all even values of n , solutions corresponding to $\omega \rightarrow \infty$ ($1/\sqrt{\omega} \rightarrow 0$), which are usually called an *asymptotic solutions*. This corresponds to the exact solution for non-interacting electrons, namely, electrons in the absence of a Coulombian potential. Our result is qualitatively different to that of Ref. [11], where it was found that those solutions exist only for odd values of n .

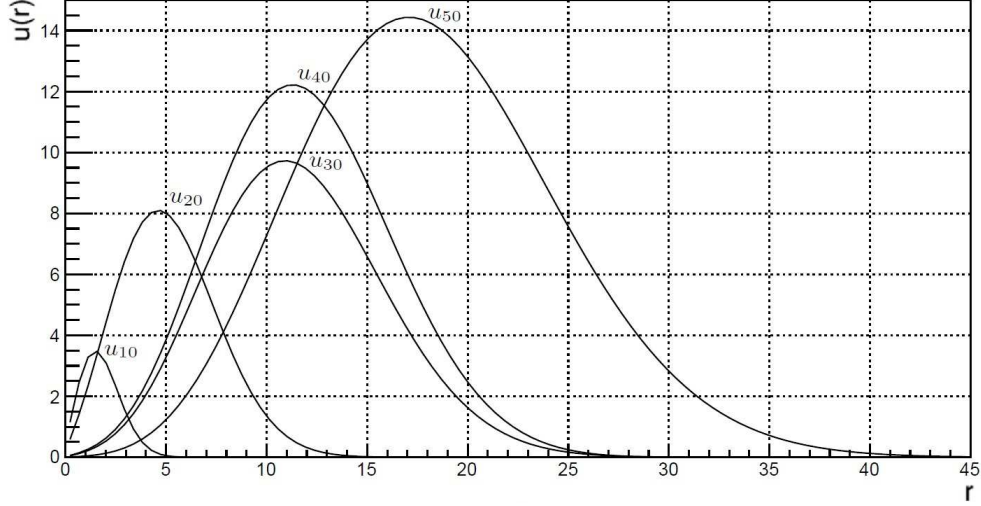


Figure 1: Radial wave function u_{nl} , for $l = 0$ and $n = 1, 2, 3, 4$, and 5 .

To see what is happening, let us choose, instead of Eq. (9), the condition

$$\gamma - \alpha - 2 = 4n$$

In this case, the Heun equation, Eq. (5), can be written as

$$x y''(x) + [1 + \alpha - 2x^2] y' + [4nx - \delta/2] y(x) = 0 \quad (10)$$

Neglecting the δ term is equivalent to the choice $1/\sqrt{\omega} \rightarrow 0$ ($\omega \rightarrow \infty$), and means exactly that non-interacting electrons are considered. In this case, the solution of Eq. (10) can be expressed in terms of the Laguerre polynomial $L_n^\alpha(x)$, as [14]

$$y(x) = n! \frac{\Gamma(1 + \alpha/2)}{\Gamma(1 + \alpha/2 + n)} L_n^{\alpha/2}(x^2)$$

which is in agreement with the result of Ref. [15].

3. Numerical results for the $1/r$ potential

It is clear from the previous Section that the solutions obtained by solving the Biconfluent Heun equation, Eq. (5), present a strong limitation. Indeed, each polynomial solution is valid just for one specific frequency. Therefore, it is difficult to compare the theoretical prediction with a particular experiment for a given external harmonic oscillator potential of frequency $\Omega = 2\omega$.

This motivates us to search for numerical solutions of the radial Schrödinger equation, Eq. (4). Such eigenvalue equation can be numerically solved by a slightly modified version of the Numerov method [12], as done in reference [13]. The algorithm was implemented in a program developed by the authors using C^{++} language. Both calculations and graphics shown in this paper were done by using the CERN/ROOT package.

The first numerical result is aimed to show the linear relation, given by Eq. (9), between the energy η_{nl} and n and l . Such linear relation was indeed found and is shown in Fig. 2 for the particular case when $l = 0$. The frequency for this numerical result was fixed as $\omega = 0.01$ Ha. Remember that since the quantum dot is submitted to a microwave external excitation, we can use values for the frequency Ω in the range $0.01 \text{ Ha} < \Omega < 1 \text{ Ha}$.

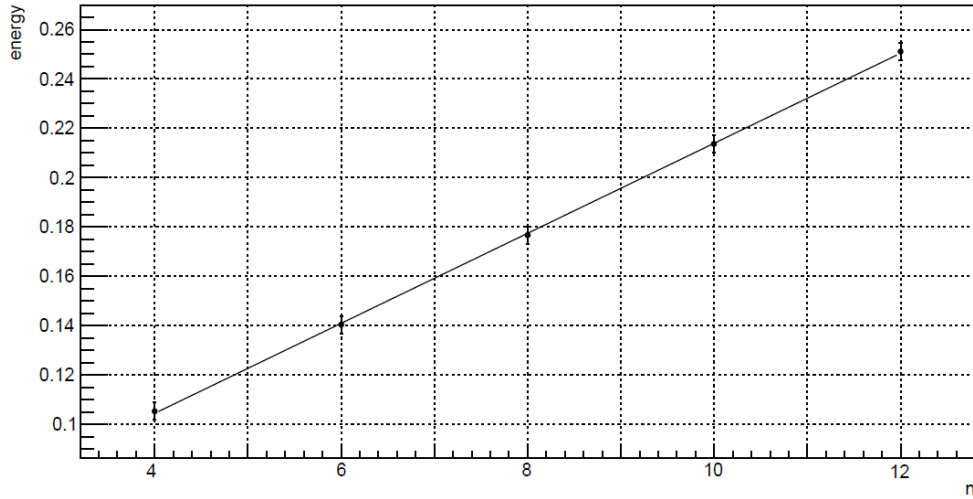


Figure 2: Linear relation between the energy and n as result from the Numerov numerical method considering $l = 0$ and $\omega = 0.01$ Ha.

Not only the general linear behavior is proved but also the particular energy values associated to different values of n were calculated and are in good agreement if compared to the analytical results of the previous Section. These results are given in Table 2.

Table 2: Comparison between analytical and numerical energy solutions for $l = 0$, $\omega = 0.01$ Ha, and different values of n .

n	η_{n0} (Ha) prediction	
	analytical	numerical
4	0.1	0.1053
6	0.14	0.1404
8	0.18	0.1767
10	0.2	0.2136
12	0.26	0.2511

The numerical eigenfunction for these states are shown in Fig. 3.

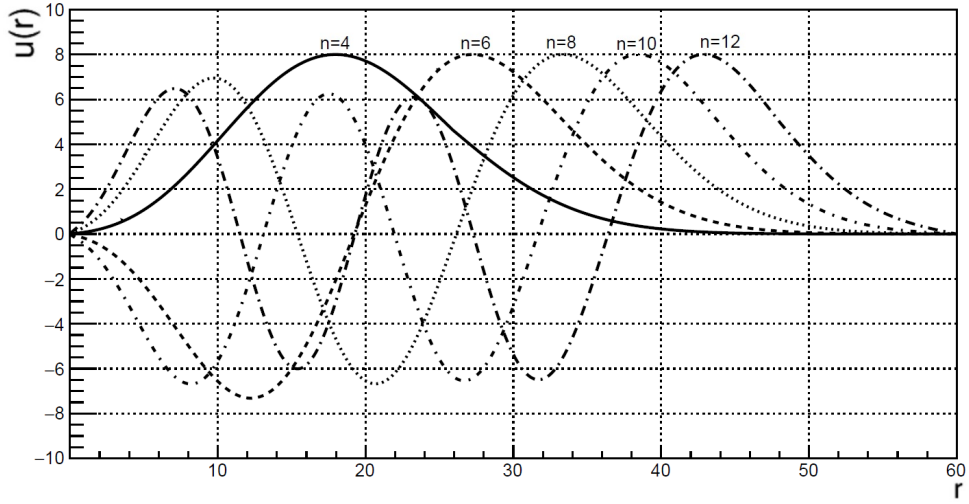


Figure 3: Numerov numerical method eigenfunctions corresponding to the choice of external frequency $\omega = 0.01$ Ha.

Another test to confirm the analytical predictions was possible by running the numerical program for the specific frequency value associated to each polynomial solution. For simplicity we give here just the comparison considering the states $l = 0$. The theoretical value of the energy, computed by Eq. (9), and the respective output from the numerical method are shown in Table 3, for $1 \leq n \leq 5$.

Table 3: Comparison between analytical and numerical energy solutions for some values of ω .

n	ω (Ha)	η_{n0} (Ha) prediction	
	frequency	analytical	numerical
1	0.5	2	2.059
2	0.083	0.492	0.4994
3	0.027	0.216	0.2162
4	0.012	0.12	0.12
5	0.022	0.264	0.2649

In Fig. 4 some theoretical polynomial eigenfunctions $u(r)$ are compared to the respective numerical function.

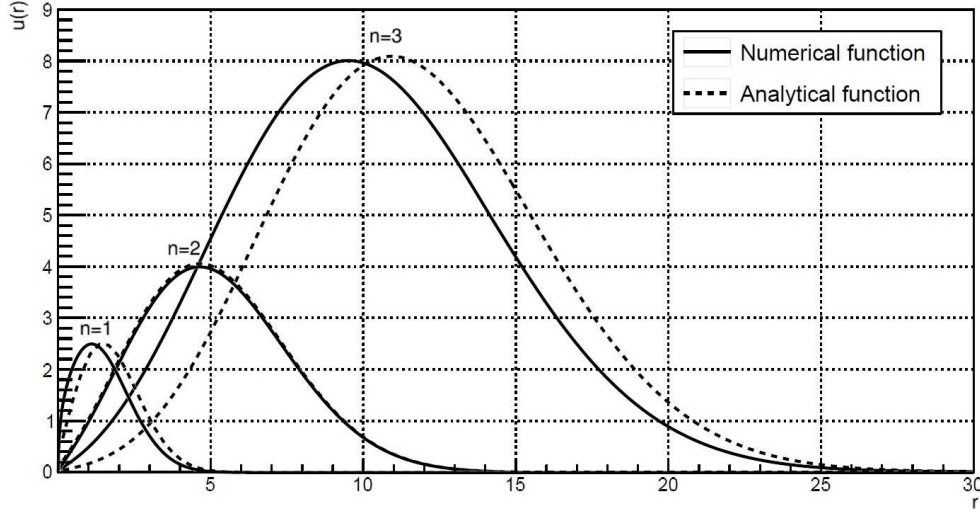


Figure 4: Eigenfunctions corresponding to some frequencies of Table 3.

4. Numerical solutions for the $\ln r$ potential

It is straightforward to solve numerically the radial equation for the quantum dot, Eq. (4), substituting the Coulombian potential $1/r$, derived from Gauss' theorem in (1+3)D by the $\ln(r)$ potential [16, 17] which is expected to be the Coulombian-like potential in (1+2)D.

We were able to find just the first two solutions with positive energies in the case of $\ln(r)$ potential. The comparison between the energy values for both potential formula is given in Table 4.

Table 4: Comparison between $1/r$ and $\ln(r)$ potentials for $\omega = 0.01$ Ha and different values of n .

n	η_{n0} (Ha) prediction	
	$1/r$	$\ln(r)$
4	0.1053	0.7107
6	0.1404	1.725
8	0.1767	-
10	0.2136	-
12	0.2511	-

The wave-functions for the first two lower states are given in Fig. 5.

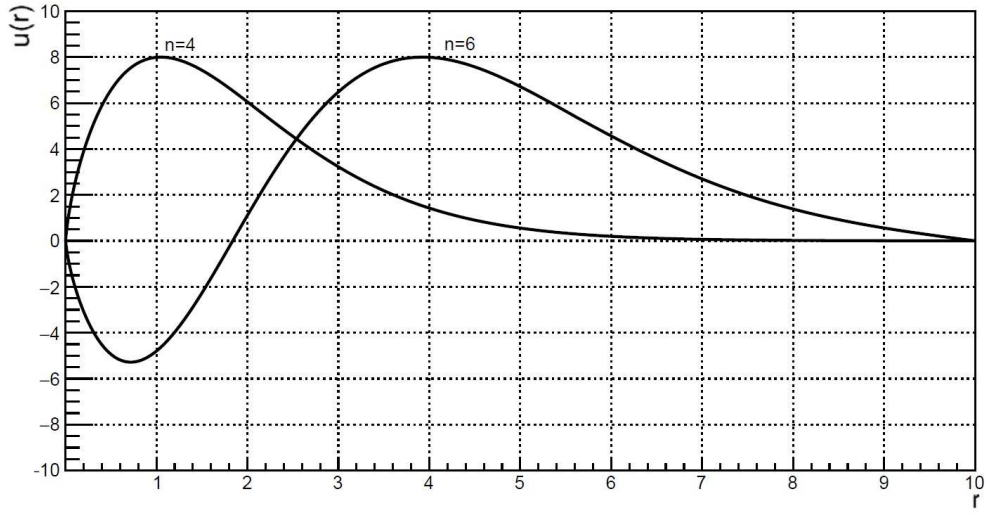


Figure 5: Eigenfunctions for the $\ln(r)$ potential with the choice of $\omega = 0.01$ Ha.

5. Bound state solutions

First of all we have to understand that in a strictly planar system bound states can exist only for $l = 0$. This peculiar fact depends on the nature

of the effective potential of Eq. (4) since, only in two spatial dimensions, the so called “centrifugal potential” becomes indeed attractive just for the value $l = 0$. Otherwise the sum of Coulombian and centrifugal potentials are always repulsive.

For each kind of potential we were able to numerically find several states. The ground state energy value is $E = -63.92$ Ha, for the $1/r$ potential, to be compared with $E = -45.92$ Ha, for the $\ln(r)$ potential. Both values are obtained with $\omega = 0.01$ Ha. However, for small values of r , the energies are not bias by the ω choice (at least in the range we are considering in this paper). If these values are compared to the ground state energy of the hydrogen atom in three dimensions, $E_H = -0.5$ Ha, we see that they differ from one order of magnitude.

The eigenfunctions corresponding to these states are given in Fig. 6.

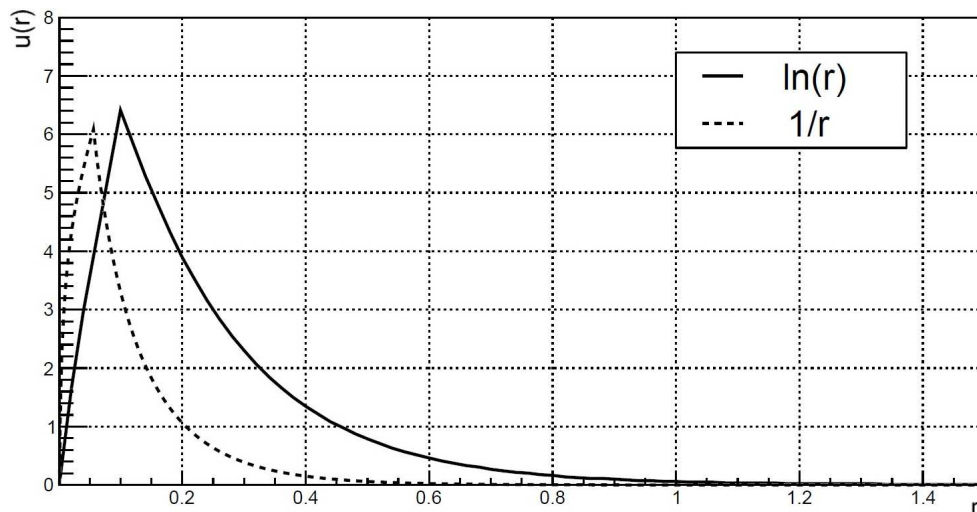


Figure 6: Comparison between wave-functions for the ground state in the case of a $\ln(r)$ and $1/r$ potentials.

6. Discussions

In this paper we present some corrections to the theoretical analysis of Ref. [8]. The new results were confronted with success with numerical calculations based on the Numerov method as show throughout the paper. One of the limitations of the polynomial solutions is the fact that each eigenvalue do

exist just for one specific value of the external frequency. Thus the comparison with experimental data is in principle a hard task. Unless it is possible to vary the external frequency Ω continuously.

This kind of restriction is no more present in the numerical calculations. Thus, in principle, we can find more than one state for a given external frequency. However, we learned that when the Numerov method is able to predict a particular state for a given frequency corresponding to an even value of n , it means that all subsequent states, for the same frequency, will correspond to other even values. If the first state is now obtained for odd n value, all other states will be associated to odd values of n .

After taking into account several comparisons between our numerical program and known results, we were confident to explore new solutions for both $1/r$ and $\ln(r)$ potentials. The first potential is strictly valid for a (1+3)D flat space-time. In spite of this fact, a very large amount of papers had discussed the two-dimensional quantum dots using this potential. This can be justified by imagining that the two-dimensional physical system is an idealization immersed in a three-dimensional world. By other side, the potential $\ln(r)$ is expected to be valid only in a (1+2)D flat space-time. Some comparisons of physical observables predicted numerically for both kind of potential were presented in Sections 4 and 5, namely, the positive energies η and the bound state energies E . The significative difference between these values can be used to shed light on the problem of space dimensionality. Indeed, we can see from Table 4, that if space is strictly two-dimensional the quantum dot energy will be one order of magnitude greater than the corresponding value got with the $1/r$ potential.

If we now consider the discrepancy of the values for the ground state which is predicted only for (1+2)D and $l = 0$ we realize that it is not so big. However, we notice that they are quite two order of magnitudes greater in modulus than the bound energy of the hydrogen atom in (1+3)D.

All this emphasize the interest in the study of two-dimensional physical systems and can be seen as a justification to pursue the investigation on the planar hydrogen atom and on planar quantum dot.

Acknowledgment

The authors are pleased to thank Bartolomeu D.B. de Figueiredo for fruitful discussions.

7. References

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